

APPLIED MATHEMATICS & MODELING FOR CHEMICAL ENGINEERS

CHAPTER ONE

Formulation of Mathematical Models

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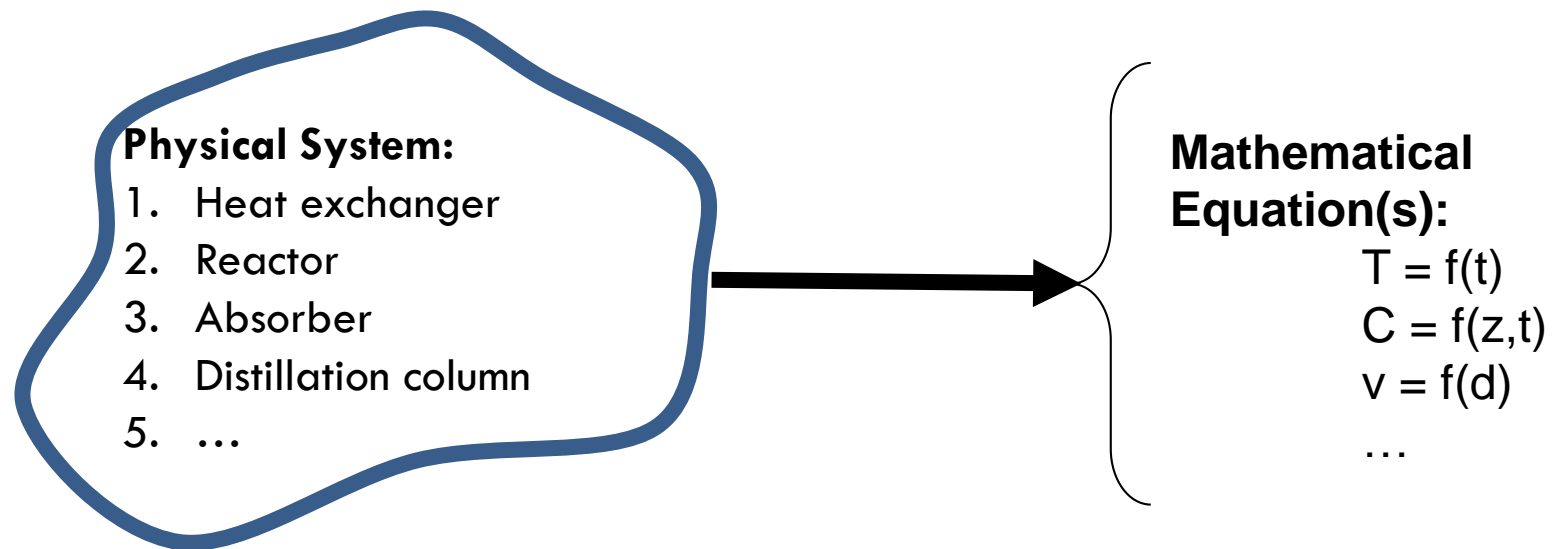
Department of Chemical Engineering



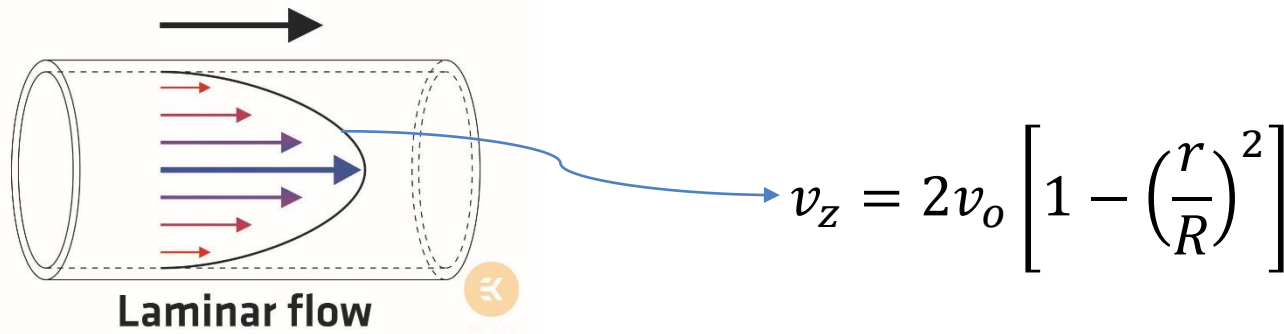
Definitions

2

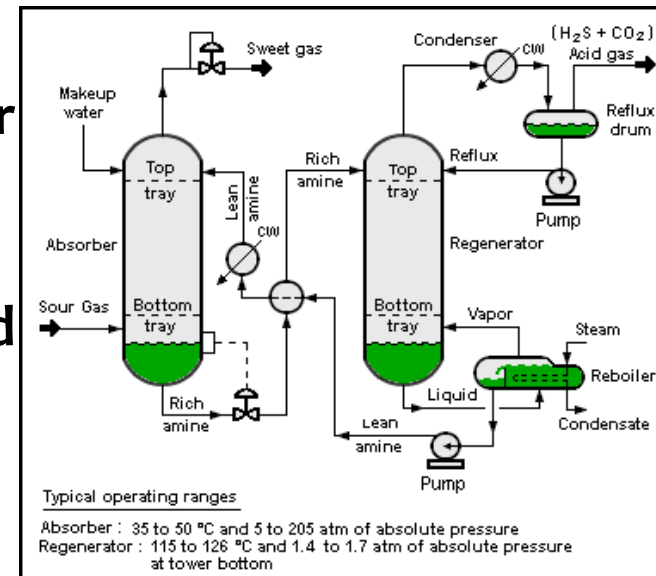
- **Process Modeling** is the mathematical representation of a physical/chemical/biological/ etc. process and/or phenomena.



- **1960: Robert Bird** introduced his textbook **Transport Phenomena**. → A textbook that is mainly based on problem formulation by elementary differential balances.



- **Developed Models and the need for programming language for coding**
 - ▣ C++ , MATLAB, Simulink, etc
- **Process simulation is the use of Models or Model-based simulators to design, develop, optimize, predicate the behaviour of single equipment/integrated process.**



Commercial Simulators



Aspen Plus®: Chemical industries

Hysys®: Gas & Oil

Honeywell

UniSim®: Gas & Oil



ChemCAD®: Chemical Industries

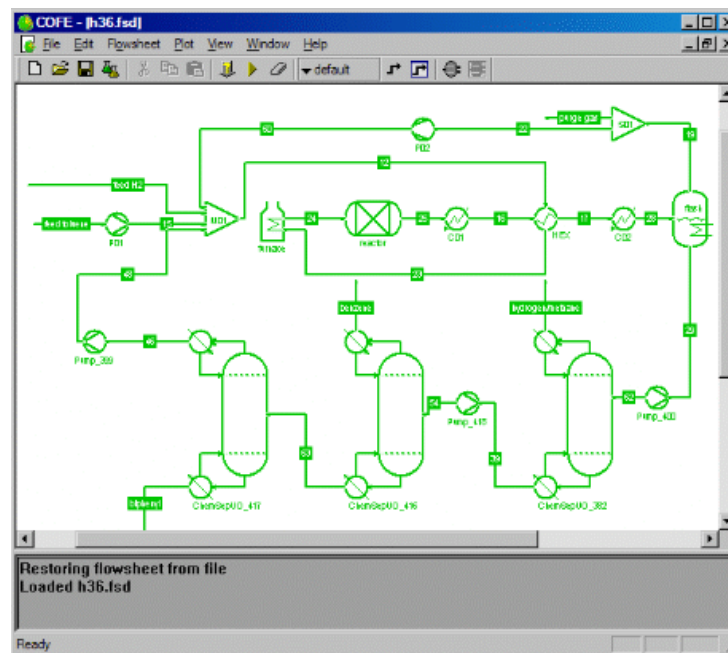
i n v e n s i s

Operations Management

PRO/II®: Chemical industries

Bryan Research & Engineering, Inc.

ProMax®: Gas & Oil



SuperProg Designer®: Batch processing
(Pharmaceuticals, water treatment...)

The Four Major Stages in Process Modeling

5

A. Problem Imagination

- Proper Understanding of the Problem
- Problem sketch

B. Model Development

- Transforming our understanding into mathematical equations:
 - ▣ Purpose of the model
 - ▣ Physical & Chemical Information
 - ▣ Conservation laws and Rate laws
 - ▣ Selecting representative differential element
 - ▣ Determining the Boundary and Initial Conditions

C. Mathematical Solution

- ☐ Analytical
- ☐ Numerical

D. Model Validation

- ☐ Experimental Data
- ☐ Operational Evidence

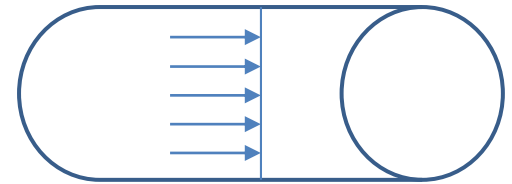
Models Development & Analysis

21

Example: Fluid Cooling

Case # 1

- Develop a model to find the temperature of a fluid flowing at steady-state in a pipe, assume that the pipe wall temperature is constant and the flow is turbulent.
- In the solution, I will assume that ΔT is not large, this implies that
- Turbulent flow implies that



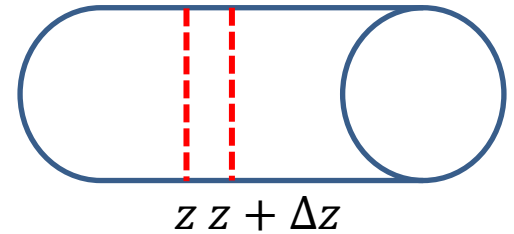
Energy Balance on the differential element:

$$E|_{in} - E|_{out} + E|_{Gen} = E|_{acc}$$

$$mc_p T|_z - mc_p T|_{z+\Delta z} - h(2\pi R \Delta z)(T - T_w) = 0.0$$

$$\lambda = \frac{2\pi R h}{mc_p}$$

$$T|_z - T|_{z+\Delta z} - \lambda \Delta z (T - T_w) = 0.0$$



Divide by Δz and take the limit:

$$\lim_{\Delta z \rightarrow 0} \frac{T_{z+\Delta z} - T_z}{\Delta z} = \frac{dT}{dz}$$

$$\therefore \frac{dT}{dz} = -\lambda(T - T_w)$$

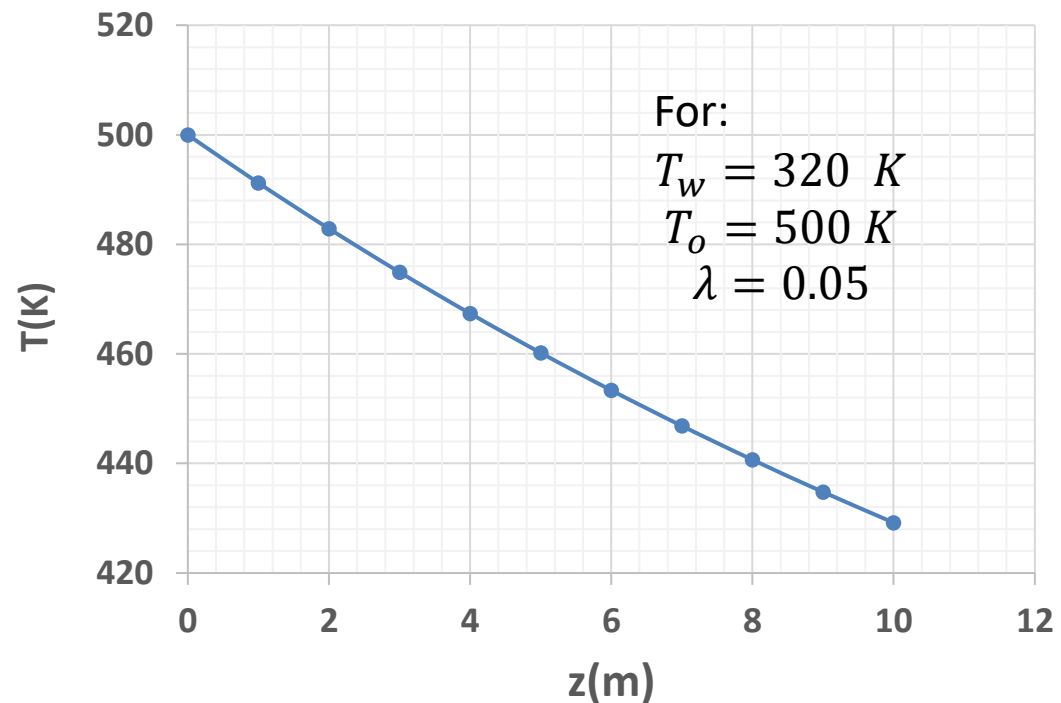
$$\frac{dT}{T - T_w} = -\lambda dz \rightarrow \int_{T_o}^T \frac{dT}{T - T_w} = \int_0^z -\lambda dz$$

$$\ln(T - T_w) \Big|_{T_o}^T = -\lambda z \Big|_0^z$$

$$\ln\left(\frac{T - T_w}{T_o - T_w}\right) = -\lambda z$$

$$\frac{T - T_w}{T_o - T_w} = \exp(-\lambda z)$$

$$T = (T_o - T_w) \exp(-\lambda z) + T_w$$



Case # 2

- Re-model the same system, but this time assume that the flow is laminar

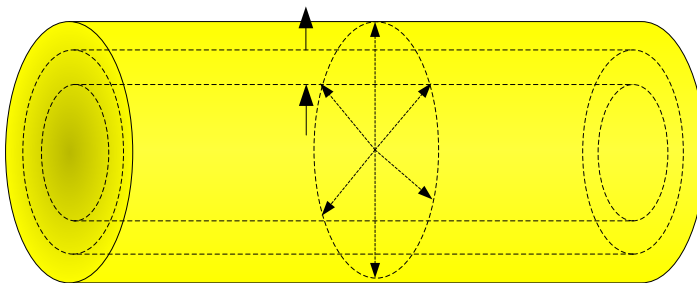
- Flow pattern consequences

- ❖ v_z is not constant in the radial direction

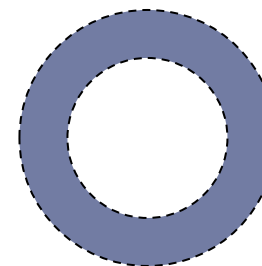
$$v_z = 2v_o \left[1 - \left(\frac{r}{R} \right)^2 \right]$$

- ❖ There will be heat conduction in the radial direction
- ❖ Convection might be small \rightarrow we have also to consider the conduction in the axial direction.

- Selection of the differential element

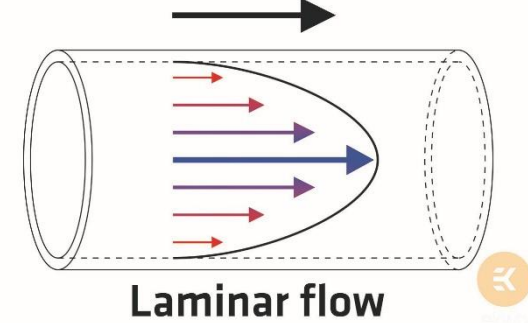


Variable changes in radial direction

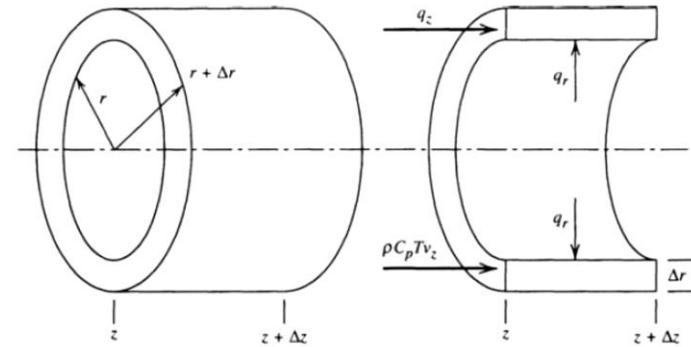


$$2\pi r \Delta r$$

Edge area



Energy balance on the differential element



$$v_z(2\pi r\Delta r)\rho c_p T \Big|_z - v_z(2\pi r\Delta r)\rho c_p T \Big|_{z+\Delta z} + (2\pi r\Delta r)q_z \Big|_z - (2\pi r\Delta r)q_z \Big|_{z+\Delta z} \\ + (2\pi r\Delta z)q_r \Big|_r - (2\pi r\Delta z)q_r \Big|_{r+\Delta r} = 0.0$$

Divide by $2\pi\Delta r\Delta z$ & take the limit

$$-v_z r \rho c_p \frac{T|_{z+\Delta z} - T|_z}{\Delta z} - \frac{r q_z|_{z+\Delta z} - r q_z|_z}{\Delta z} - \frac{r q_r|_{r+\Delta r} - r q_r|_r}{\Delta r} = 0.0$$

$$-v_z r \rho c_p \frac{\partial T}{\partial z} - \frac{\partial(r q_z)}{\partial z} - \frac{\partial(r q_r)}{\partial r} = 0.0$$

Divide by r & rearrange

$$v_z \rho c_p \frac{\partial T}{\partial z} + \frac{\partial q_z}{\partial z} + \frac{1}{r} \frac{\partial(r q_r)}{\partial r} = 0.0$$

We know that

$$q_r = -k \frac{\partial T}{\partial r} \quad \text{And} \quad q_z = -k \frac{\partial T}{\partial z}$$

$$v_z \rho c_p \frac{\partial T}{\partial z} - \frac{\partial \left(k \frac{\partial T}{\partial z} \right)}{\partial z} - \frac{1}{r} \frac{\partial \left(r k \frac{\partial T}{\partial r} \right)}{\partial r} = 0.0$$

$$2v_o \left[1 - \left(\frac{r}{R} \right)^2 \right] \left(v_z \rho c_p \frac{\partial T}{\partial z} \right) = k \frac{\partial^2 T}{\partial z^2} + \frac{k}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right)$$

Boundary Conditions

$$z = 0 \text{ \& } r = r \rightarrow T(0, r) = T_o$$

$$z = \infty \text{ \& } r = r \rightarrow T(\infty, r) = T_w$$

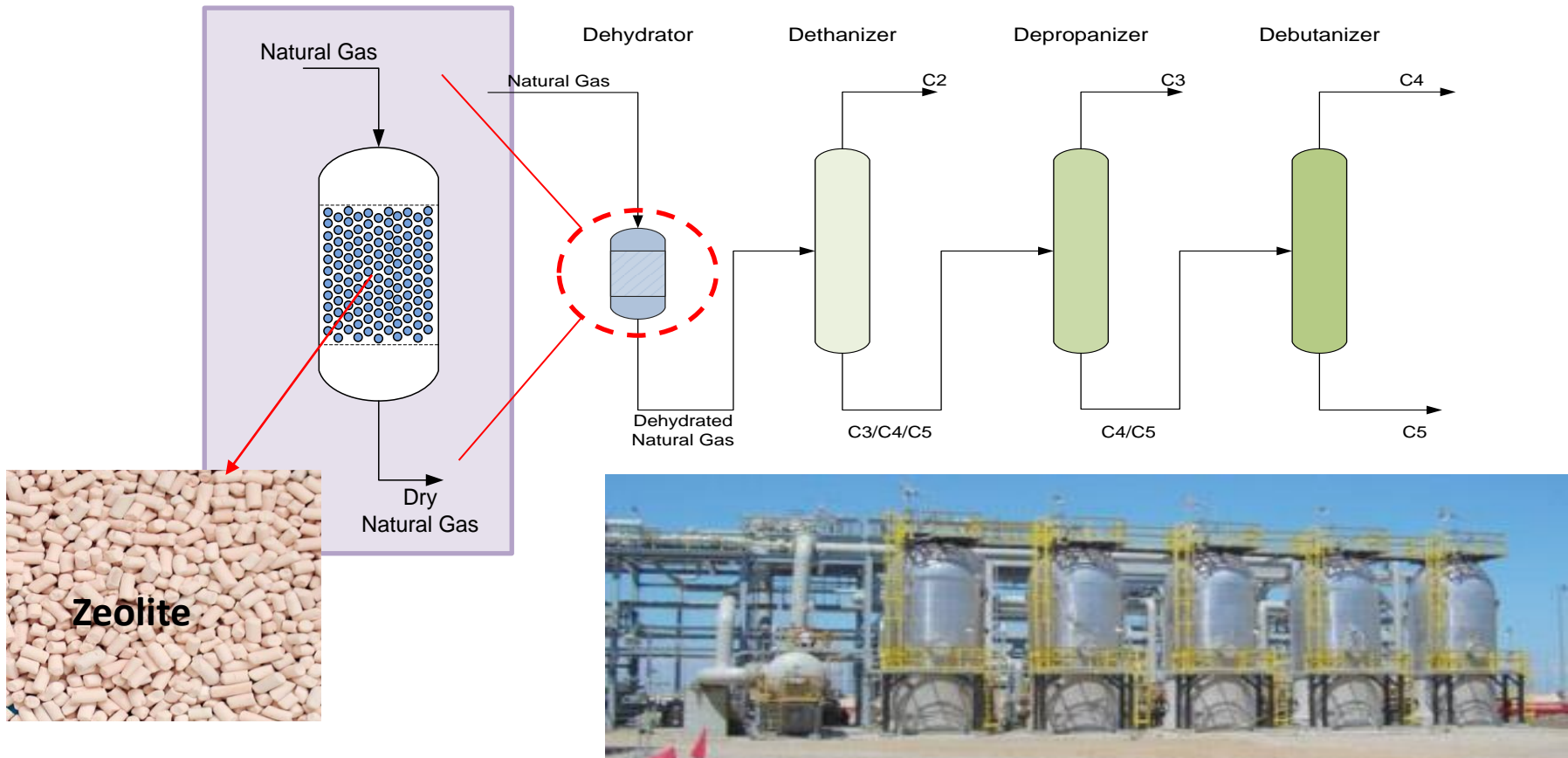
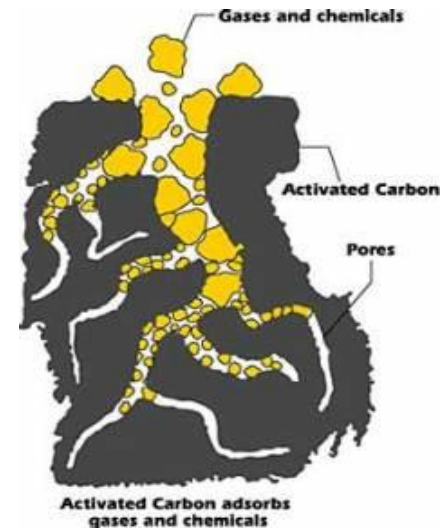
$$z = z \text{ \& } r = R \rightarrow T(z, R) = T_w$$

$$z = z \text{ \& } r = r \rightarrow \frac{\partial T}{\partial r} = 0$$

$$T(z, r) = \dots$$

Example: Adsorption Bed

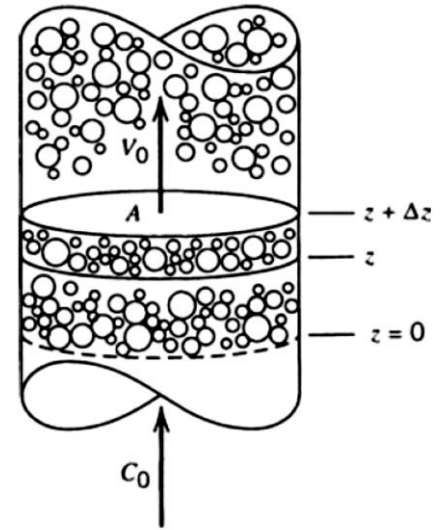
- ❑ L-S or G-S separation
- ❑ Could be chemical or physical, what is the difference?
- ❑ Activated Carbon is a good adsorbent, why?



❑ Objective: Develop a model to find the concentration of the adsorbate within the adsorption bed as function of time and location?

❑ The model to be developed based on:

- ❑ A differential element $A_c \Delta z$
- ❑ Isothermal operation
- ❑ Flat velocity profile ($v_o = \text{constant}$)
- ❑ No axial diffusion



Balance on the adsorbate

$$v_o A_c c \Big|_z - v_o A_c c \Big|_{z+\Delta z} = \varepsilon A_c \Delta z \frac{\partial c}{\partial t} + (1 - \varepsilon) A_c \Delta z \frac{\partial q}{\partial t}$$

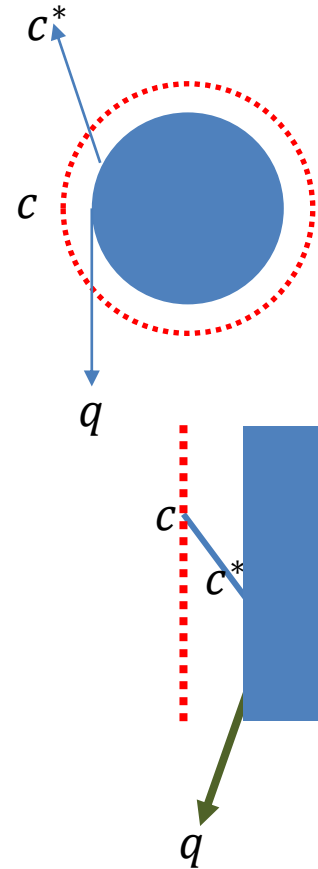
Divide by $A_c \Delta z$ and take the limit

$$-v_o \frac{\partial c}{\partial z} = \varepsilon \frac{\partial c}{\partial t} + (1 - \varepsilon) \frac{\partial q}{\partial t}$$

Based on the interfacial equilibrium

$$q = Kc^*$$

$$-v_o \frac{\partial c}{\partial z} = \varepsilon \frac{\partial c}{\partial t} + (1 - \varepsilon)K \frac{\partial c^*}{\partial t} \dots\dots\dots (1)$$



Balance on the solid phase:

$$k_c a A_c \Delta z (c - c^*) = A_c \Delta z (1 - \varepsilon) \frac{\partial q}{\partial t}$$

Divide by $A_c \Delta z$ and use $q = Kc^*$

$$k_c a (c - c^*) = (1 - \varepsilon)K \frac{\partial c^*}{\partial t} \dots\dots\dots (2)$$

Boundary and Initial Conditions

$$z = z \text{ \& } t = 0 \rightarrow c^*(z, 0) = 0$$

$$z = z \text{ \& } t = 0 \rightarrow c(z, 0) = 0$$

$$z = 0 \text{ \& } t = t \rightarrow c(0, t) = c_o$$

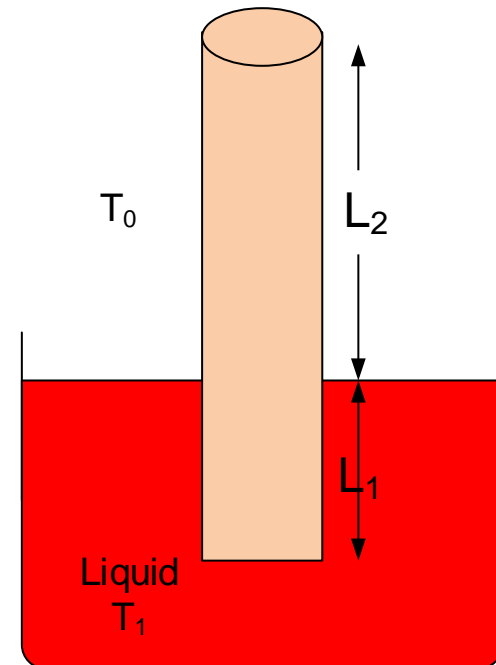
Model Details

30

- **Objective:** Estimating the heat removal from a solvent bath by a rod.
- **General Assumptions:**
 - ▣ Ignore heat transfer at rod ends
 - ▣ Overall heat transfer coefficient is constant
 - ▣ No solvent evaporation
 - ▣ The system is at st.st.

Level # I

Assume the rod temperature is uniform inside and outside the solvent (i.e. no temperature gradient in the radial or axial directions)



Energy balance around the rod

$$E \Big|_{in} = E \Big|_{out}$$

$$h_L(2\pi RL_1)(T_1 - T) = h_G(2\pi RL_2)(T - T_o)$$

Divide by $2\pi R$

$$h_L L_1 T_1 - h_L L_1 T = h_G L_2 T - h_G L_2 T_o$$

$$h_L L_1 T_1 + h_G L_2 T_o = h_G L_2 T + h_L L_1 T$$

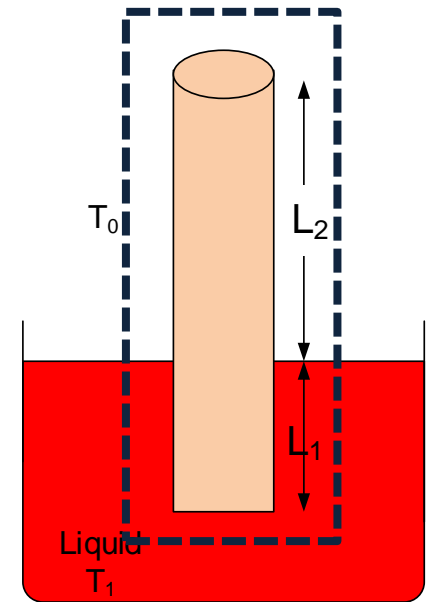
Solve for T

$$T = \frac{h_L L_1 T_1 + h_G L_2 T_o}{h_G L_2 + h_L L_1}$$

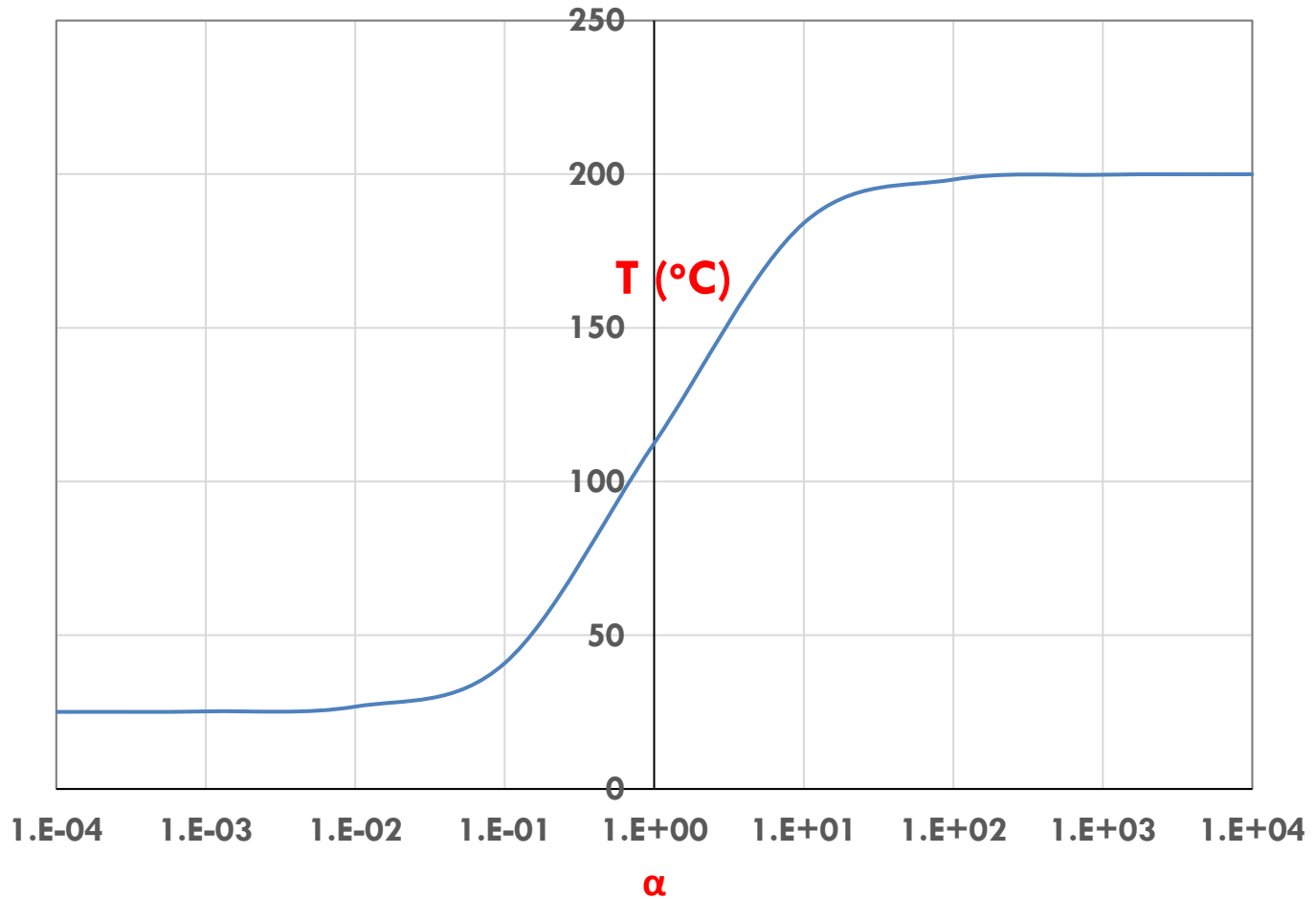
Define α

$$\alpha = \frac{h_L L_1}{h_G L_2}$$

$$\rightarrow T = \frac{\alpha T_1 + T_o}{1 + \alpha}$$

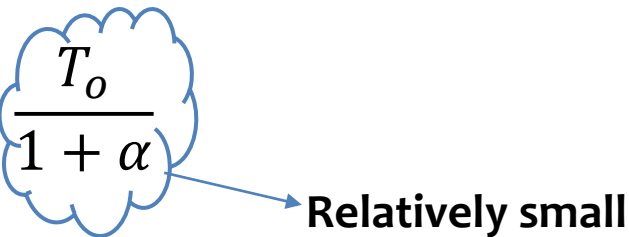


Temperature of the rod as function of α for a system at
 $T_1 = 200^\circ\text{C}$ and $T_o = 25^\circ\text{C}$



if $\alpha \gg 1$

$$T = \frac{\alpha T_1 + T_o}{1 + \alpha} = \frac{\alpha T_1}{1 + \alpha} + \frac{T_o}{1 + \alpha}$$

$$\rightarrow T = T_1 + \frac{T_o}{1 + \alpha}$$


Relatively small

This means that the temperature of the rod is very close to the temperature of the liquid

Rate of heat transfer

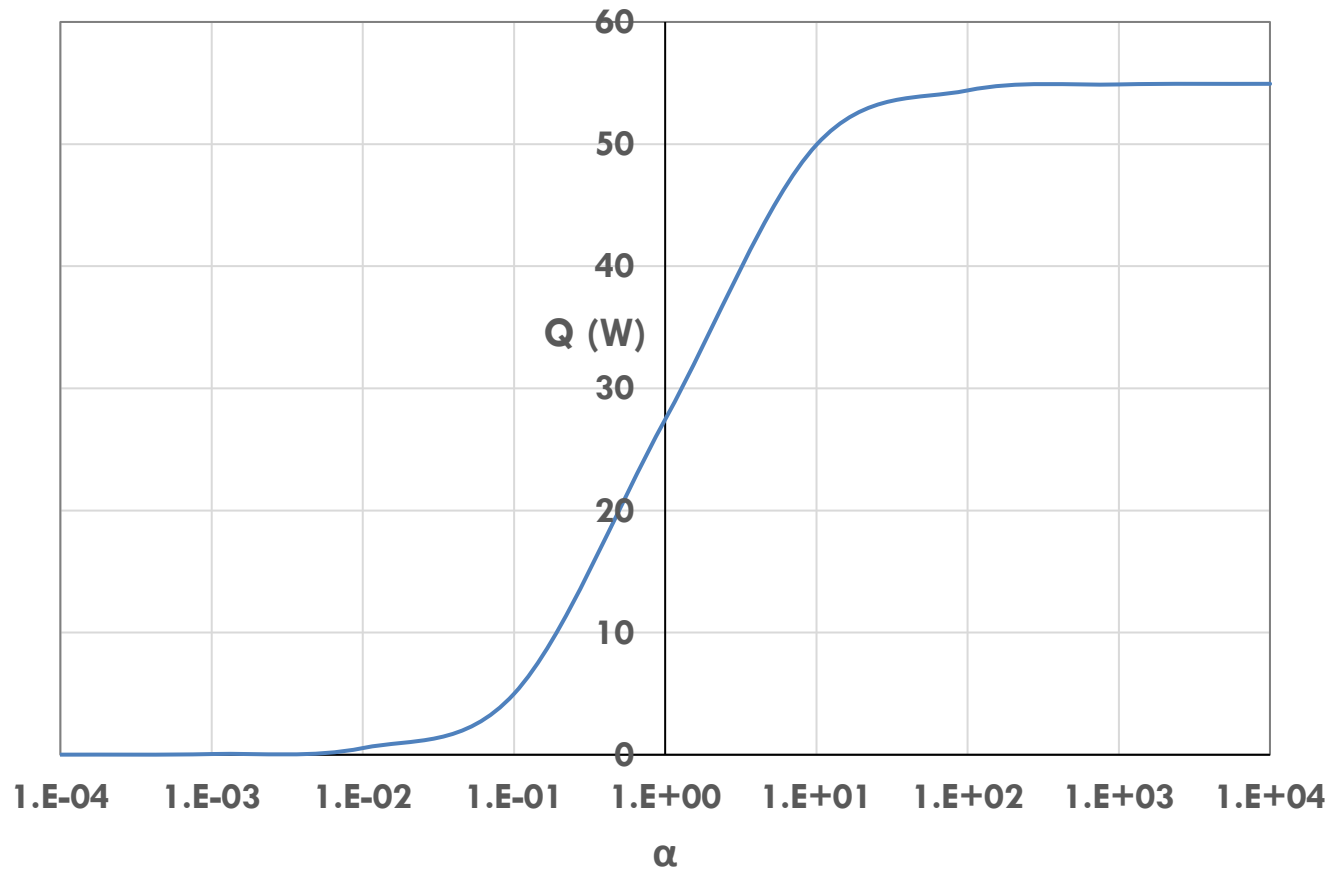
$$Q = h_G(2\pi RL_2)(T - T_o)$$

$$\text{if } \alpha \gg 1 \rightarrow T \cong T_1$$

$$Q \cong h_G(2\pi RL_2)(T_1 - T_o)$$

Heat loss from the system as function of α for a system at

$$T_1 = 200\text{ }^{\circ}\text{C}, T_o = 25^{\circ}\text{C}, h_G = 10 \frac{\text{W}}{\text{m}^2 \cdot \text{K}}, R = 0.05\text{ m and } L_2 = 0.1\text{ m}$$



Level # 2

- **The same as Level # 1, but at this level we will assume that:**
 - ▣ The temperature of the rod in the liquid is uniform and equals the temperature of the liquid.
 - ▣ The temperature of the rod outside the liquid is not uniform in the axial direction.

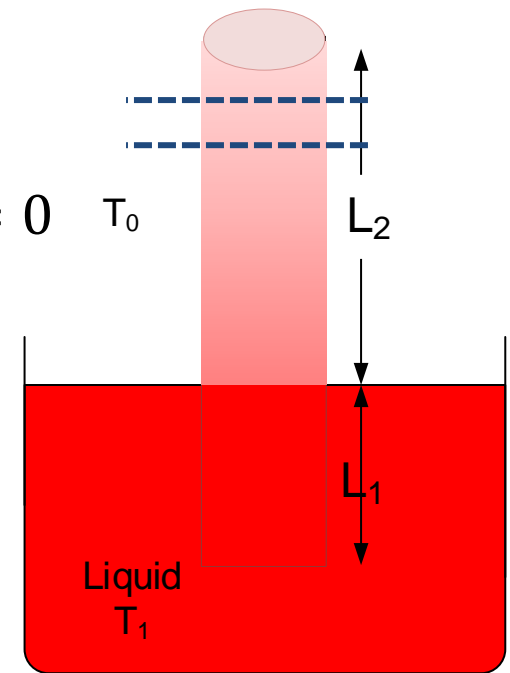
Energy balance on the differential element

$$\pi R^2 q \Big|_x - \pi R^2 q \Big|_{x+\Delta x} - h_G (2\pi R \Delta x) (T - T_o) = 0 \quad T_o$$

Divide by $\pi R^2 \Delta x$ And take the limit

$$-\frac{dq}{dx} - \frac{2h_G}{R} (T - T_o) = 0$$

But $q = -k \frac{dT}{dx}$



$$k \frac{d^2 T}{dx^2} = \frac{2h_G}{R} (T - T_o)$$

- ODE
- 2nd Order
- Non-homogeneous

Boundary Conditions:

$$x = 0 \rightarrow T = T_1$$

$$x = L_2 \rightarrow \left. \frac{dT}{dx} \right|_{L_2} = 0$$

$$\frac{d^2 T}{dx^2} - \lambda(T - T_o) = 0$$

$$\lambda = \frac{2h_G}{kR}$$

$$\theta = T - T_o$$

$$d\theta = dT \quad \& \quad d^2\theta = d^2T$$

$$\frac{d^2\theta}{dx^2} - \lambda\theta = 0$$

$$m^2 - \lambda = 0 \rightarrow m = \pm\sqrt{\lambda}$$

$$\theta(x) = A \cosh(\sqrt{\lambda}x) + B \sinh(\sqrt{\lambda}x)$$

1st BC

$$x = 0 \rightarrow T = T_1 \rightarrow \theta = T_1 - T_o$$

$$T_1 - T_o = A \cosh(0) + B \sinh(0)$$

$$\rightarrow A = T_1 - T_o$$

2nd BC

$$x = L_2 \rightarrow \left. \frac{dT}{dx} \right|_{L_2} = 0 \rightarrow \left. \frac{d\theta}{dx} \right|_{L_2} = 0$$

$$\frac{d\theta}{dx} = A\sqrt{\lambda} \sinh(\sqrt{\lambda}x) + B\sqrt{\lambda} \cosh(\sqrt{\lambda}x)$$

$$\rightarrow 0 = (T_1 - T_o)\sqrt{\lambda} \sinh(\sqrt{\lambda}L_2) + B\sqrt{\lambda} \cosh(\sqrt{\lambda}L_2)$$

$$\rightarrow B = -\frac{(T_1 - T_o) \sinh(\sqrt{\lambda}L_2)}{\cosh(\sqrt{\lambda}L_2)}$$

$$\theta(x) = (T_1 - T_o)\cosh(\sqrt{\lambda}x) - \frac{(T_1 - T_o)\sinh(\sqrt{\lambda}L_2)}{\cosh(\sqrt{\lambda}L_2)}\sinh(\sqrt{\lambda}x)$$

$$T(x) - T_o = (T_1 - T_o)\cosh(\sqrt{\lambda}x) - (T_1 - T_o)\tanh(\sqrt{\lambda}L_2)\sinh(\sqrt{\lambda}x)$$

$$T(x) = T_o + (T_1 - T_o)\cosh(\sqrt{\lambda}x) - (T_1 - T_o)\tanh(\sqrt{\lambda}L_2)\sinh(\sqrt{\lambda}x)$$

For $k \gg h_G \rightarrow \lambda \ll 1$ and $x = L_2$

$$T(L_2) = T_o + (T_1 - T_o)\cosh(\sim 0) - (T_1 - T_o)\tanh(\sim 0)\sinh(\sim 0)$$

$$T(L_2) = T_o + (T_1 - T_o) - (T_1 - T_o)(0)$$

$$T(L_2) = T_1$$

Compare to level 1

For $k \ll h_G \rightarrow \lambda \gg 1$ and $x = L_2$

$$T(L_2) = T_o + (T_1 - T_o)\cosh(\sqrt{\lambda}L_2) - (T_1 - T_o)\tanh(\sqrt{\lambda}L_2)\sinh(\sqrt{\lambda}L_2)$$

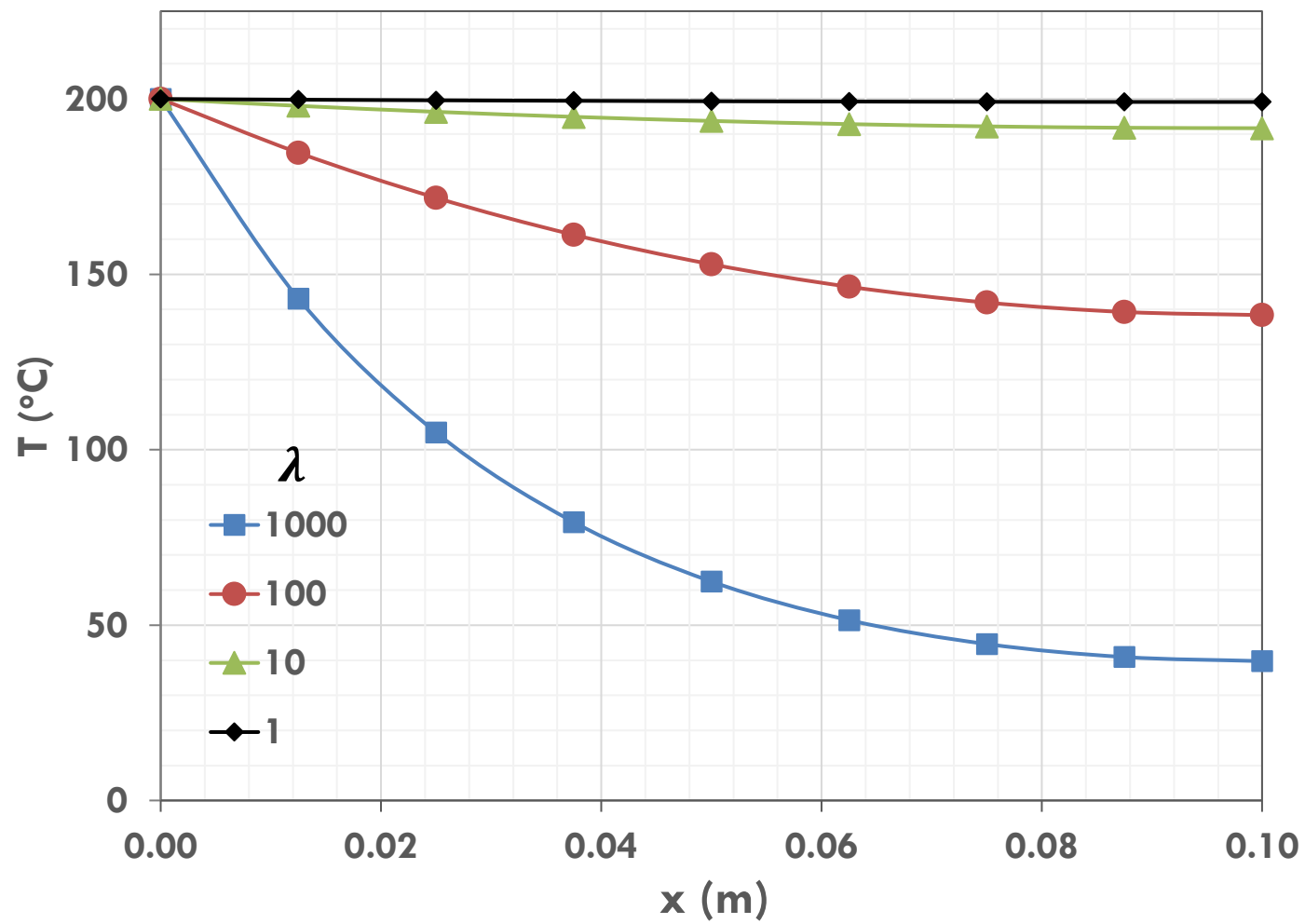
$$T(L_2) = T_o + (T_1 - T_o)\cosh(\sqrt{\lambda}L_2) - \frac{(T_1 - T_o)\sinh(\sqrt{\lambda}L_2)}{\cosh(\sqrt{\lambda}L_2)}\sinh(\sqrt{\lambda}L_2)$$

$$T(L_2) = T_o + (T_1 - T_o) \left(\frac{\cosh(\sqrt{\lambda}L_2)\cosh(\sqrt{\lambda}L_2) - \sinh(\sqrt{\lambda}L_2)\sinh(\sqrt{\lambda}L_2)}{\cosh(\sqrt{\lambda}L_2)} \right)$$

$$T(L_2) = T_o + (T_1 - T_o) \left(\frac{1}{\cosh(\sqrt{\lambda}L_2)} \right)$$

Very small

$$\rightarrow T(L_2) = T_o$$



Rate of heat transfer

$$\text{Option \#1} \quad Q = -k\pi R^2 \left. \frac{dT}{dx} \right|_{x=0}$$

$$\frac{dT}{dx} = (T_1 - T_o)\sqrt{\lambda}\sinh(\sqrt{\lambda}x) - (T_1 - T_o)\sqrt{\lambda}\tanh(\sqrt{\lambda}L_2)\cosh(\sqrt{\lambda}x)$$

$$\left. \frac{dT}{dx} \right|_{x=0} = (T_1 - T_o)\sqrt{\lambda}\sinh(0) - (T_1 - T_o)\sqrt{\lambda}\tanh(\sqrt{\lambda}L_2)\cosh(0)$$

$$\left. \frac{dT}{dx} \right|_{x=0} = -(T_1 - T_o)\sqrt{\lambda}\tanh(\sqrt{\lambda}L_2)$$

$$\rightarrow Q = k\pi R^2 (T_1 - T_o)\sqrt{\lambda}\tanh(\sqrt{\lambda}L_2) \quad \times \frac{\sqrt{\lambda}L_2}{\sqrt{\lambda}L_2}$$

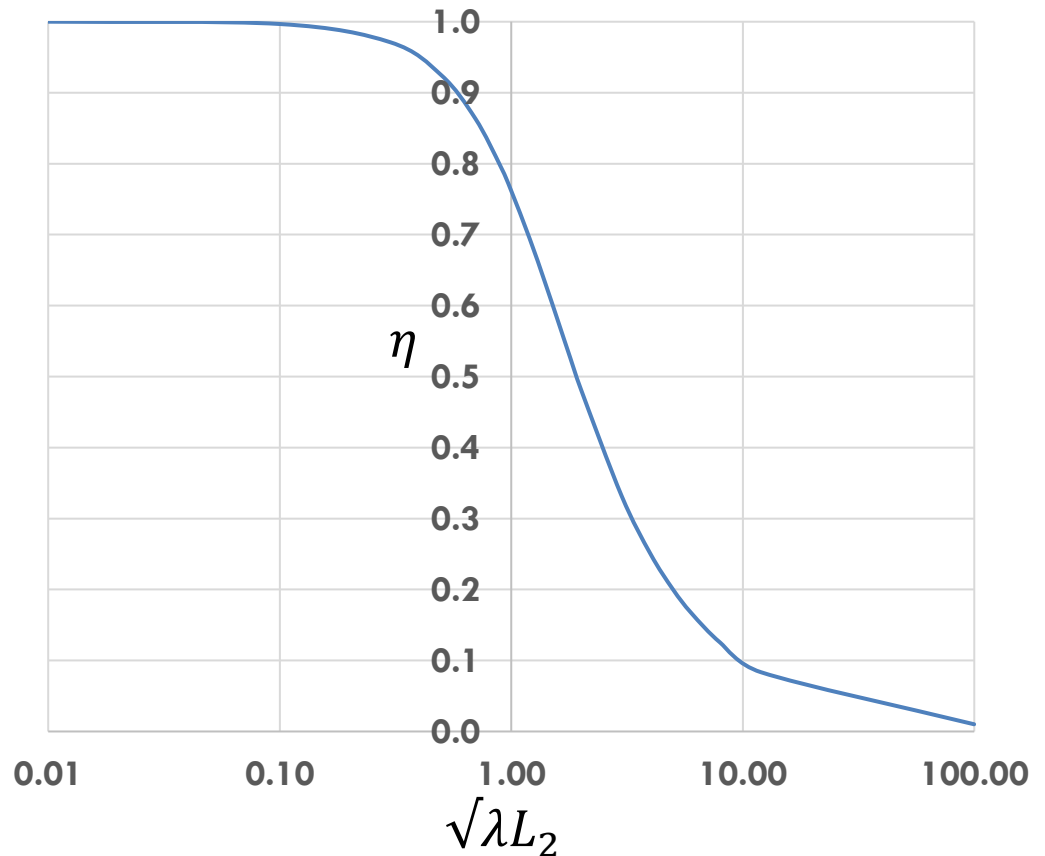
$$Q = k\pi R^2 (T_1 - T_o)\lambda L_2 \frac{\tanh(\sqrt{\lambda}L_2)}{\sqrt{\lambda}L_2}$$

$$Q = k\pi R^2 (T_1 - T_o) \left(\frac{2h_G}{Rk} \right) L_2 \frac{\tanh(\sqrt{\lambda}L_2)}{\sqrt{\lambda}L_2}$$

$$\therefore Q = (2\pi RL_2)h_G(T_1 - T_o) \frac{\tanh(\sqrt{\lambda}L_2)}{\sqrt{\lambda}L_2}$$

Effectiveness factor

$$\eta = \frac{\tanh(\sqrt{\lambda}L_2)}{\sqrt{\lambda}L_2}$$



Option #2

$$Q = \int_0^{L_2} h_G(2\pi R)(T - T_o)dx$$

Function of x

Level # 3

At this level we will keep the same previous assumptions except that there are temperature gradients in the rod within the liquid and within the gas phase.

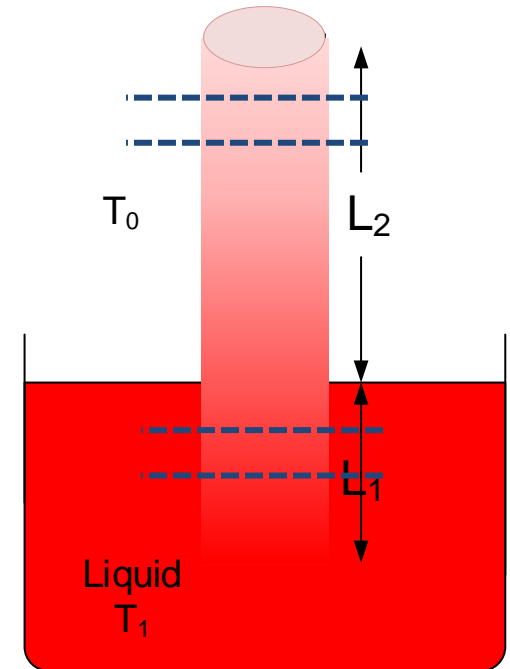
T_L : Temperature of the rod in the lower part

T_U : Temperature of the rod in the upper part

We have to develop 2 models, one for the upper section of the rod and one for the lower section

$$k \frac{d^2 T_L}{dx^2} = \frac{2h_L}{R} (T_L - T_1)$$

$$k \frac{d^2 T_U}{dx^2} = \frac{2h_U}{R} (T_U - T_o)$$



Boundary Conditions

$$x = -L_1 \rightarrow \frac{dT_L}{dx} = 0$$

$$x = L_2 \rightarrow \frac{dT_U}{dx} = 0$$

$$x = 0 \rightarrow T_L = T_U$$

$$x = 0 \rightarrow \left. \frac{dT_L}{dx} \right|_{x=0} = \left. \frac{dT_U}{dx} \right|_{x=0}$$

Solution

$$T_L = T_1 + A \cosh(n(x + L_1))$$

$$T_U = T_o + B \cosh(m(L_2 - x))$$

$$n = \sqrt{\frac{2h_L}{Rk}}$$

$$m = \sqrt{\frac{2h_G}{Rk}}$$

$$A = \frac{-(T_1 - T_o)}{\cosh(nL_1) + \frac{n}{m} \frac{\sinh(nL_1)}{\sinh(mL_2)} \cosh(mL_2)}$$

$$B = \frac{(T_1 - T_o)}{\cosh(mL_2) + \frac{m}{n} \frac{\sinh(nL_1)}{\sinh(mL_2)} \cosh(mL_2)}$$

Rate of heat transfer

$$Q = -\pi R^2 k \left. \frac{dT_L}{dx} \right|_{x=0}$$

$$T_L = T_1 + A \cosh(n(x + L_1))$$

$$\frac{dT_L}{dx} = nA \sinh(n(x + L_1))$$

$$\left. \frac{dT_L}{dx} \right|_{x=0} = nA \sinh(n(0 + L_1)) = nA \sinh(nL_1)$$

$$Q = -\pi R^2 k n A \sinh(nL_1)$$

$$Q = -\pi R^2 k n \sinh(nL_1) \frac{-(T_1 - T_o)}{\cosh(nL_1) + \frac{n}{m} \frac{\sinh(nL_1)}{\sinh(mL_2)} \cosh(mL_2)}$$

Divide by $\sinh(nL_1)$

$$Q = \pi R^2 k n \frac{(T_1 - T_o)}{\frac{\cosh(nL_1)}{\sinh(nL_1)} + \frac{n}{m} \frac{\cosh(mL_2)}{\sinh(mL_2)}}$$

$$Q = \pi R^2 k n \frac{(T_1 - T_o)}{\frac{1}{\tanh(nL_1)} + \frac{n}{m} \frac{1}{\tanh(mL_2)}}$$

Multiply by: $\frac{m}{n} \tanh(mL_2) / \frac{m}{n} \tanh(mL_2)$

$$Q = \pi R^2 k m \frac{(T_1 - T_o) \tanh(mL_2)}{\frac{m \tanh(mL_2)}{n \tanh(nL_1)} + 1} \quad \text{Multiply by: } \frac{mL_2}{mL_2}$$

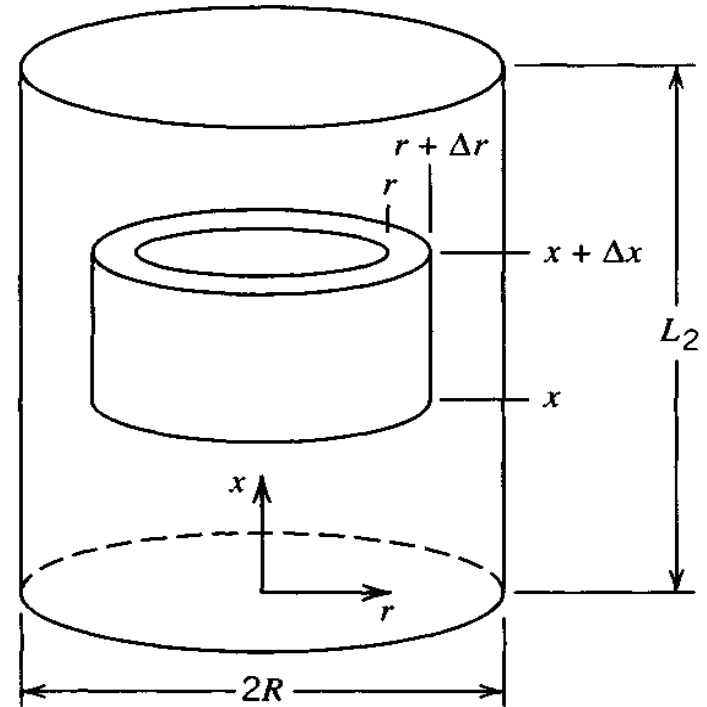
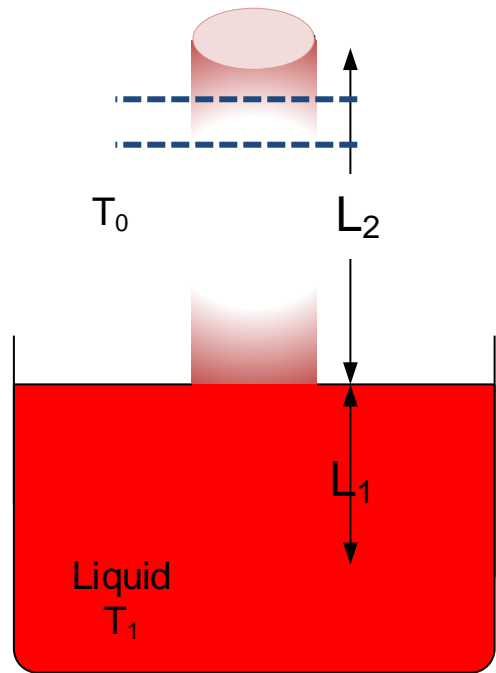
$$Q = \pi R^2 k \boxed{m^2} L_2 \frac{(T_1 - T_o)}{\frac{m \tanh(mL_2)}{n \tanh(nL_1)} + 1} \frac{\tanh(mL_2)}{mL_2}$$

$m^2 = \lambda = \frac{2h_G}{Rk}$
 η

$$Q = h_G (2\pi R L_2) \eta \frac{T_1 - T_o}{1 + \left(\frac{m \tanh(mL_2)}{n \tanh(nL_1)} \right)}$$

Level # 4

At this level we will consider the heat flux in the radial direction for the upper section.



$$(2\pi r \Delta r) q_x \Big|_x - (2\pi r \Delta r) q_x \Big|_{x+\Delta x} + (2\pi r \Delta x) q_r \Big|_r - (2\pi r \Delta x) q_r \Big|_{r+\Delta r} = 0$$

Divide by $2\pi \Delta r \Delta x$ and take the limit

$$-\frac{\partial(rq_x)}{\partial x} - \frac{\partial(rq_r)}{\partial r} = 0.0$$

$$q_r = -k \frac{\partial T}{\partial r} \qquad q_x = -k \frac{\partial T}{\partial x}$$

$$kr \frac{\partial^2 T}{\partial x^2} + k \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) = 0.0$$

$$k \left(\frac{\partial^2 T}{\partial x^2} + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) \right) = 0.0$$

Boundary Conditions:

$$r = 0 \text{ and } x = x \rightarrow \frac{\partial T}{\partial r} \Big|_{r=0} = 0$$

$$r = R \text{ and } x = x \rightarrow -k \frac{\partial T}{\partial r} = h_G (T - T_o)$$

$$r = r \text{ and } x = 0 \rightarrow T = T_1$$

$$r = r \text{ and } x = L_2 \rightarrow \frac{\partial T}{\partial x} = 0$$

⋮

$$Q = \frac{2\pi R^2 k (T_1 - T_o)}{L_2 \Delta} \sum_{n=1}^{\infty} \frac{\beta_n < 1, K_n >^2}{< K_n, K_n >} \tanh\left(\frac{\beta_n}{\Delta}\right)$$

$$Bi = \frac{h_G R}{k}$$

When $Bi \ll 1$

$$\therefore Q = (2\pi R L_2) h_G (T_1 - T_o) \eta$$

Boundary Conditions

51

□ Homogenous BCs

$$y(x) = 0 \quad @ x = x_o$$

$$\left. \frac{dy}{dx} \right|_{x=x_o} = 0 \quad @ x = x_o$$

$$\beta y + \frac{dy}{dx} = 0 \quad @ x = x_o$$

□ Nonhomogeneous BCs

$$y(x) = \alpha \quad @ x = x_o$$

□ Nonhomogeneous BCs can be transferred to homogenous BCs

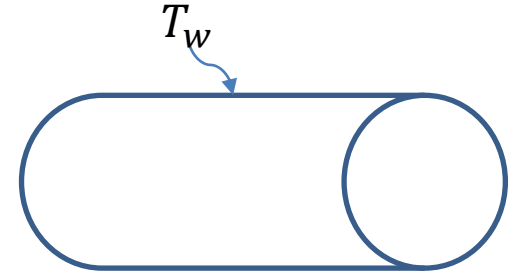
Example

Convert the following nonhomogeneous BCs into homogenous BCs

$$a) T(z, R) = T_w$$

$$\text{Assume } \theta = T - T_w$$

$$\rightarrow \theta(z, R) = T_w - T_w = 0$$



$$b) \text{ if at } r = R \quad -k \frac{dT}{dr} = U(T - T_c)$$

$$\text{Assume } \theta = T - T_c$$

$$-k \frac{d\theta}{dr} = U\theta \Rightarrow \frac{U}{k}\theta + \frac{d\theta}{dr} = 0$$

